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Effectiveness of Different Artificial Neural Network Models in Establishing the Suitable Dosages of Coagulant and Chlorine in Water Treatment Works

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ABSTRACT

Generally, in India, determining the chlorine and coagulant dosage in a WTP depends on the proficiency of operators, which may lead to overdosing or underdosing of coagulants and chlorine. Nevertheless, the determination of both coagulant and chlorine dosages frequently changes as inlet water quality varies which demands extensive laboratory analyses, leading to prolonged experimentation periods in water treatment plants. So objective of the study is to develop the precise relationship between coagulant dose and chlorine dose in a water treatment plant by using an artificial neural network (ANN). As a result, ANN models were developed to predict chlorine dose using coagulant dose by comparing the performance of the number of ANN models. It has been found that radial basis function neural networks (RBFNN) and generalized regression neural networks (GRNN) modeling provide better prediction. In RBFNN and GRNN modeling, the spread factor is varied from 0.1 to 15 to establish a stable and accurate model with high predictive accuracy. It is observed that the RBFNN model showed good prediction (R^2 = 0.999). The application of a soft computing model for defining doses of coagulant and chlorine that are inextricably linked at a Water treatment plant (WTP) will be highly beneficial for WTP Managers.

INTRODUCTION

In WTP, there are various treatment processes but the most important nonlinear and complex treatment processes are coagulation and disinfection because they ensure safe and clear water. Generally, chlorine is the most commonly used disinfectant, and aluminum sulfate (alum) is a coagulant due to its ease of application, monitoring, low cost, and effectiveness. The effectiveness of the chlorination and coagulation process mainly depends upon three major parameters, namely turbidity of water, pH of water, and applied dosages (Bello et al. 2014, Bowden et al. 2006). Traditionally, optimum coagulant doses are determined using jar tests. However, jar tests are conducted periodically, which means that they are reactive rather than proactive, whereas coagulant doses need to change continuously with turbidity (Bobadilla et al. 2019, Chan Moon 2017). In India, generally, in WTP coagulant dose is kept constant for specific periods due to a time delay of the jar test, which leads to the production of a dose or overdose of coagulant sometimes. Chlorine emerges as the dominant disinfectant due to its ease of application and monitoring, low cost, and strong bactericidal capabilities. The efficacy of chlorination is heavily dependent on three key parameters: water turbidity, pH levels, and the amount of chlorine applied (Constans et al. 2003, Librantz et al. 2018).

Turbidity plays a vital role in both coagulation and disinfection processes, facilitating particle settlement and acting as a shield against microbes (Kennedy et al. 2018). However, the relationship between turbidity, chlorination, and coagulation demonstrates nonlinear behavior, proving challenging to capture through linear mathematical models (Kim & Kim 2014). Hence, there arises a necessity to devise prediction models for residual chlorine utilizing Artificial Neural Networks (ANNs).

Traditionally, in India, determining chlorine dosage in a WTP relies on operators' expertise, while coagulant dosage is assessed through jar tests (Haghiri et al. 2017). However, the determination of both coagulant and chlorine dosages typically involves labor-intensive laboratory analyses, leading to prolonged experimental times in field water treatment plants (Kejiang et al. 2013). Consequently, there is a pressing need to develop predictive models for chlorine dosage based on coagulant dosage at WTPs. Such models would streamline the dosage determination process, enhancing efficiency and ensuring optimal water treatment outcomes.

In this study, many ANN models for the establishment of the relationship between the Coagulant and Chlorine Dose are developed. It is necessary to test and compare various ANN and training algorithms to develop a network that can perform satisfactorily in a reasonable amount of time (Jayaweera & Aziz 2018). Each model is trained many times, and the best performance is evaluated.

MATERIALS AND METHODS

For Coagulant and chlorine dose neural network (CCDNN) modeling, 1849 data samples of input variables (Turbidity of the outlet water, residual chlorine, and coagulant dose) and target variable (chlorine dose) were collected from WTP. The variables examined in this study are inextricably linked to the coagulation and chlorination processes. Data were collected from the WTP laboratory for four years for inlet and outlet water quality daily (2012-2016). MATLAB version 16 was used to develop ANN models. ANN models such as RBFNN, FFNN, CFNN, and GRNN have been developed with a trial run that allows modification of the input variables, hidden nodes, training function, and the spread factor (SF). It is always a difficult task to create an optimal number of hidden nodes in ANN applications (Reilly et al. 2018, Salim & Noureddine 2015, Loc et al. 2020). The optimum number of nodes in each layer is not possible precisely and easily. In this study, information from both input and output nodes is used for building hidden neurons in a hidden layer. The training and test data are divided between 75:30 and 80:20, respectively, during the development of the ANN models. Diverse training functions, such as Bayesian Regularization (BR), Levenberg-Marquartz (LM), Resilient Back Propagation (RP), BFGS Quasi-Newton (BFG), One-Step Secant (OSS) Conjugated Gradient Back Propagation (CGB), Cluster-Powell (CGF), and Gradient Back Propagation (VLRB) are used. It was reported that the RBFNN and the GRNN models have the best test performance, respectively, with SF of 1 and 0.1 (Heddam et al. 2011). Thus, RBFNN and GRNN models ranging from 0.1 to 15 have been tested in this study. Standard statistics (JK), a standard deviation (L), skewness (M1), kurtosis (M2), and error statistics like regression coefficient (R), mean square error (MSE) and mean absolute error are used to quantify the percentage performance of these ANN models (MAE) (Alka & Dnyaneshwar 2019). For its highest R and lowest MSE and MAE values, the best-performing ANN model is chosen. In addition, standard statistics, time series plots, and scatterplots are checked for the mapping with the observed series. For the best model in each category, GUIs for chlorine prediction and coagulant dosage were developed.

RESULTS AND DISCUSSION

Neural Network Model for Coagulant and Chlorine Dose 1

Sixteen models are developed for the coagulant and chlorine dose neural network 1 (CCDNN1) model. To establish the optimal networks, coagulant dose as the input parameter and chlorine dose as the output parameter are examined with various training functions and ANN. Based on numerous performance criteria, the behavior of ANNs is evaluated which is shown in Table 1.

For ANN prediction with FFNN and CFNN, different training functions were tried with varying hidden nodes from 15 to 90 (Alka & Dnyaneshwar 2019), and for RBFNN and GRNN, the value of SF varied from 0.1 to 20 during training to achieve the best-performing network. It is observed during the training period that minimum MSE = 0.019 and minimum MAE = 0.078 whereas maximum value of R^2 = 0.753 is found. Similarly, standard statistics σ = 0.137 to 0.873, ɣ1 = -2.058 to 0.635, and ɣ2 = 1.978 to 15.718. During training, it is observed that as SF value decreases in GRNN and RBFNN models, the values of R increase and values of MSE decrease. On the other hand, predictions are highly comparable RBFNN 1 model with SF = 0.1.

Similarly, it is observed during the testing period the minimum MSE = 0.014 and minimum MAE = 0.068, whereas the maximum value of R^2 = 0.715 is found. Similarly, standard statistics such as σ = 0.12 to 0.608, ɣ1 = -2.461 to-0.762, and ɣ2 = 3.184 to 12.287.

Prediction accuracy is higher for the RBFNN1 model with SF = 0.1 obtained. Further performance measures of all models are compared and observed that all the models resulted in poor performance, only the RBFNN1 model produced a good result (R = 0.72). Fig.1. shows the plot of observed and predicted series of best FFNN, CFNN, RBFNN, and GRNN models during the testing period.

Neural Network Model for Coagulant and Chlorine Dose 2

In the coagulant and chlorine dose neural network 2 (CCDNN2) model, sixteen models are developed for the

Table 1: Performance indices of CCDNN1 models during the testing period.

Type of ANN Model	SF/Training algorithm	Error statistics			Standard statistics			
		R^2	MSE	MAE	$\bar{x}$ (1.954)	σ (0.171)	ɣ1 (2.53)	ɣ2 (12.39)
RBFNN1	0.1	0.753	0.018	0.077	1.962	0.120	-2.438	12.287
	1	0.504	0.033	0.113	1.926	0.180	-2.023	15.283
	5	0.285	0.040	0.133	1.916	0.200	-2.058	13.280
	10	0.443	0.617	0.647	1.890	0.786	0.374	2.183
	15	0.421	0.631	0.661	1.913	0.795	0.414	2.147
GRNN1	0.1	0.554	0.534	0.584	1.885	0.731	0.352	2.431
	1	0.451	0.611	0.642	1.888	0.782	0.401	2.177
	5	0.424	0.633	0.663	1.980	0.796	0.506	2.134
	10	0.385	0.660	0.699	1.929	0.812	0.593	2.073
	15	0.342	0.684	0.720	1.888	0.827	0.619	2.024
FFNN	LM	0.427	0.628	0.651	1.903	0.792	0.392	2.181
	BR	0.400	0.648	0.646	1.910	0.803	0.473	2.288
	BFG	0.396	0.649	0.672	1.9064	0.805	0.386	2.298
	RP	0.384	0.655	0.677	1.8063	0.809	0.475	2.100
	CGF	0.398	0.657	0.684	1.8038	0.810	0.406	2.191
	CGM	0.302	0.715	0.702	1.921	0.844	0.516	2.171
	OSS	0.197	0.763	0.753	1.908	0.873	0.403	2.258
CFNN	LM	0.407	0.640	0.654	1.962	0.800	0.463	2.249
	BR	0.411	0.638	0.665	1.934	0.799	0.449	2.147
	BFG	0.219	0.731	0.742	1.879	0.855	0.6351	1.980
	RP	0.237	0.724	0.732	1.914	0.851	0.631	1.978
	CGF	0.256	0.717	0.731	1.862	0.847	0.623	1.983
	CGM	0.373	0.665	0.689	1.880	0.815	0.586	2.088
	OSS	0.405	0.642	0.666	1.985	0.801	0.452	2.165

coagulant and chlorine dose neural network 2 (CCDNN1) model. To establish the optimal networks, coagulant dose, and residual chlorine as input parameters and chlorine dose as output parameters are examined with various training functions and ANN. Based on numerous performance criteria, the behavior of ANNs is evaluated. It is observed that during the training period, MSE = 0.002 to 0.028 and MAE = 0.013 to 0.104, whereas R^2 varies from 0.197 to 0.978. Similarly, standard statistics such as σ = 0.044 to 0.184, ɣ1 = -2.713 to -4.286, and ɣ2 = 19.83 to 62.15 Prediction accuracy is higher for the RBFNN2 model with SF = 0.1 obtained.

Similarly, it is observed during the testing period that minimum MSE = 0.001, and minimum MAE = 0.015, whereas the maximum value of R^2 =0.97 is found. Similarly, standard statistics such as σ = 0.036 to 0.128, ɣ1 = -1.713 to -8.717, and ɣ2 = 17.667 to 89.15. It is seen from the results of the training and testing period that the RBFNN2 model with SF = 0.1 resulted consistently better than the FFNN, CFNN, and GRNN models. Fig. 2 shows the plot of the observed and predicted series of best FFNN, CFNN, RBFNN, and GRNN models during the testing period.

Neural Network Model for Coagulant and Chlorine Dose 3

In the coagulant and chlorine dose neural network 3 (CCDNN3) model, sixteen models were developed. To establish the optimal networks, turbidity of the outlet water, residual chlorine, and coagulant dose as input parameters and chlorine dose as output parameters are examined with FFNN, CFNN, RBFNN, and GRNN. The developed models were tested to get an appropriate network that provided satisfactory performance. The important performance indices of all ANN models are displayed in Table 2, indicating standard statistics and error statistics during the testing period. From Table 2, it has been observed that during the testing period, standard statistics, for example, σ (Min) = 0.026, ɣ1 (Max) = 1.032, and ɣ2 (Min) = 5.309. Similarly, error statistics such as MSE (min) = 0.001 and MAE (min) = 0.009, whereas the

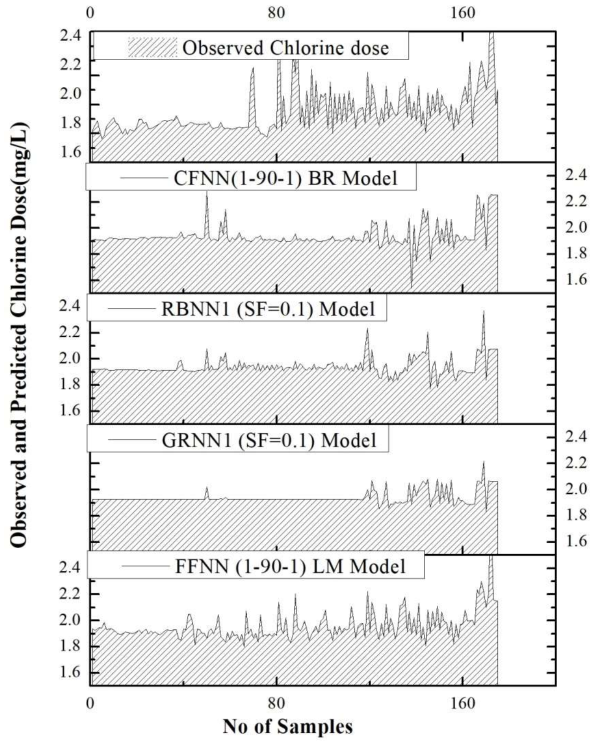

Fig. 1: Comparison of best CCDNN1 models during the testing period.

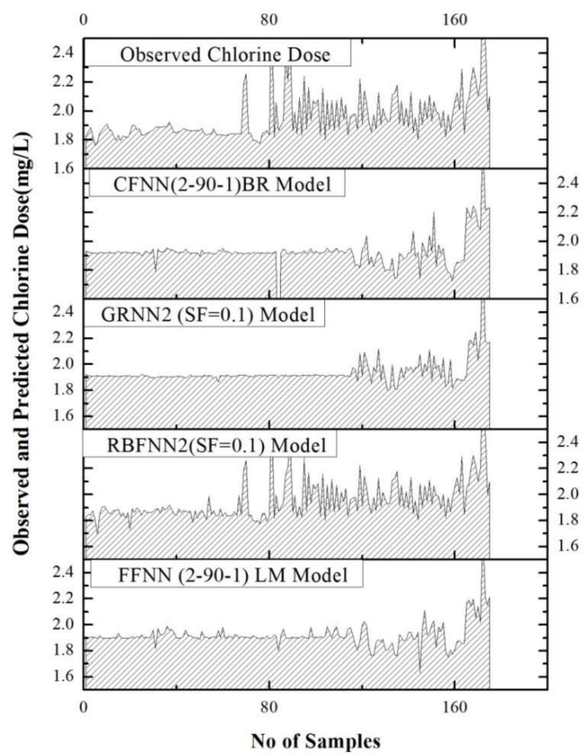

Fig. 2: Comparison of best CCDNN2 models during the testing period.

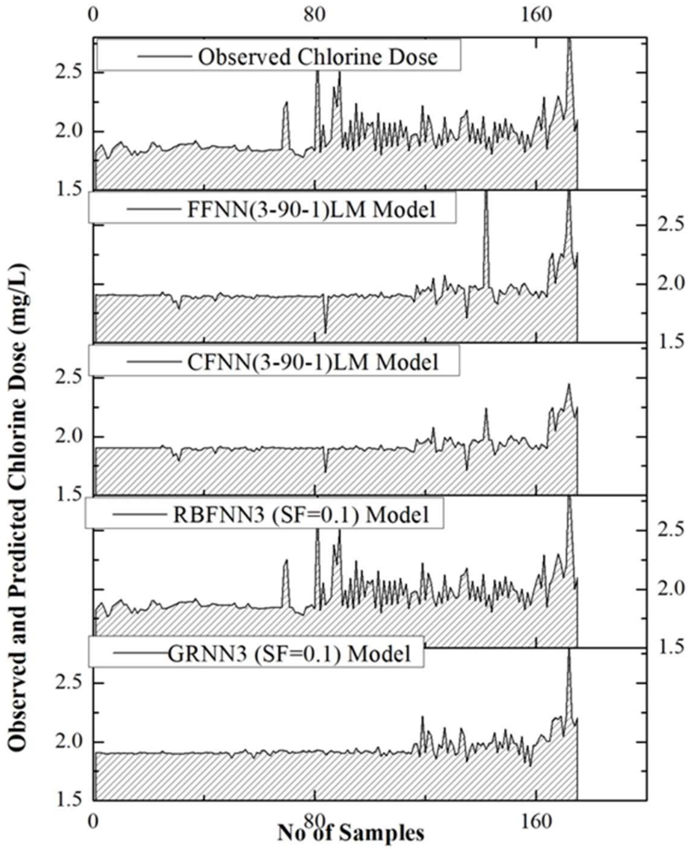

Fig. 3: Comparison of best CCDNN3 models during the testing period.

maximum value of R^2 =0.99 is found. In RBFNN and GRNN models, as SF increases, prediction efficiency decreases. In the RBFNN model, however, there is clear superiority in prediction with SF = 0.1.

Fig. 3 shows a comparison of the best CCDNN3 models in the test period, where the plot of RBFNN3 almost coincides with the plot of observed values. Compared to all other ANN models, the RBFNN3 model with SF 0.1 produced the highest R. It is found that the prediction efficiency has increased in RBFNN and GRNN models, with a decrease in SF value. Furthermore, compared to all other training algorithms, FFNN and CFNN models with BR training function produced good predictions. These models, however, are less efficient.

RBFNN models, on the other hand, have a noticeable advantage in prediction. It also demonstrates that models with three inputs perform better than models with various input variations to the networks. Tables 2 show a summary of standard statistics for the best RBFNN models in Class I, II, and III during the training and testing period. Standard statistics for all ANN models were evaluated and displayed in Table 3 during the training and testing periods. During training and testing, the RBFNN 3 model exhibited the least σ and ɣ2. Most of the best ANN models produced a positive kurtosis, where heavier tails are associated with a higher peak.

The σ (least) of the RBFNN 3 model suggests that the data points tend to be close to the set's predicted value, whereas the σ (Max) of the RBFNN 1 model indicates that data points are dispersed throughout a larger range of values.

The results of model simulation indicate that the lower the absolute value of ɣ1 (1.032), and the larger the ɣ2 (21.046) lies with RBFNN3 models, which indicate higher the accuracy of the prediction. Compared to other ANN models from Class I, II, and III, the RBFNN3 model performed the best with MSE = 0.001 and R = 0.999 over the testing period shown in Fig. 4. Time series plots and scatter plots of the RBFNN3 model during the testing period are shown in Fig. 4.a) and b), respectively. The observed and predicted chlorine dose series is seen to closely map indicating the best model. Due to better non-linear approximation, the RBFNN model showed excellent predictive results.

In most developing countries, the chlorine dose in a WTP is usually calculated by the operator's knowledge, while a

Table 2: Performance indices of CCDNN3 models during the testing period.

Type of ANN Model	SF/ Training algorithm	Error statistics			Standard statistics			
		R^2	MSE	MAE	x̄ (1.954)	σ (0.171)	ɣ1 (2.53)	ɣ2 (12.39)
RBFNN3	0.1	0.999	0.001	0.009	1.953	0.026	1.032	21.046
	1	0.812	0.01	0.047	1.949	0.1	-3.014	20.019
	5	0.012	1.069	0.298	1.853	1.005	-10.24	15.45
	10	-0.175	0.091	0.272	1.782	0.181	-2.265	12.225
	15	-0.237	0.181	0.391	1.771	0.22	-1.608	7.813
GRNN3	0.1	0.477	0.023	0.099	1.91	0.151	-2.324	11.231
	1	0.053	0.051	0.199	1.851	0.138	-3.786	28.395
	5	0.053	0.051	0.199	1.851	0.138	-3.786	28.395
	10	0.246	0.028	0.113	1.894	0.166	-2.539	12.257
	15	0.053	0.051	0.199	1.852	0.138	-3.786	28.395
FFNN	LM	0.444	0.025	0.1	1.911	0.154	-1.963	10.019
	BR	0.271	0.037	0.108	1.867	0.188	-3.107	20.4
	BFG	0.392	1.028	0.982	1.889	0.519	-1.922	6.269
	RP	0.349	0.046	0.145	1.901	0.184	-1.337	6.873
	CGF	0.407	0.033	0.119	1.918	0.166	-1.122	8.197
	CGB	0.239	0.063	0.177	1.889	0.192	-1.035	5.309
	OSS	0.262	0.037	0.117	1.899	0.186	-2.306	11.735
CFNN	LM	0.277	0.125	0.324	1.878	0.193	-2.178	10.786
	BR	0.314	0.099	0.287	1.898	0.182	-2.263	12.078
	BFG	0.32	0.143	0.344	1.888	0.212	-1.681	8.283
	RP	0.249	0.074	0.187	1.889	0.234	-1.003	4.76
	CGF	0.433	0.035	0.124	1.896	0.164	-1.133	8.628
	CGB	0.378	0.041	0.135	1.898	0.194	-0.51	9.123
	OSS	0.376	0.052	0.157	1.882	0.19	-1.136	9.387

Table 3: Standard statistics of RBFNN models during the training and testing period.

ANN Model	Training period				Testing period			
	x̄	σ	ɣ1	ɣ2	x̄	σ	ɣ1	ɣ2
Observed values	1.909	0.2088	2.0978	12.314	1.954	0.171	2.533	12.390
RBFNN1 SF = 0.1	1.910	0.137	-1.967	15.718	1.962	0.120	-2.438	12.287
RBFNN2 SF = 0.1	1.910	0.044	-4.286	62.155	1.954	0.036	-1.713	17.667
RBFNN3 SF = 0.1	1.910	0.026	3.027	98.898	1.953	0.026	2.032	21.046

jar test measures the coagulant dose. Laboratory analysis is usually used to determine the coagulant and chlorine dosage, which takes a long time in WTP. As a result, at WTP, a link between chlorine dose and coagulant dose must be established. Operators of WTP will be able to use the developed relationship to select the optimum dose.

Similarly, the relation between chlorine dose and coagulant dose is quite simplified by various n^{th} degree expressions, as shown in eq. 1, 2 and 3.

$$y = -0.00046 \times z + 1.6 \quad \ldots(1)$$

$$y = 3.5 \times 10^{-6} \times z^2 - 0.001 \times z + 1.9. \quad \ldots(2)$$

$$y = -3.5 \times 10^{-8} \times z^3 + 1.4 \times 10^{-5} \times z^2 - 0.0017 \times z + 1.9. \quad \ldots(3)$$

Where y = chlorine dose and z = coagulant dose in mg/L.

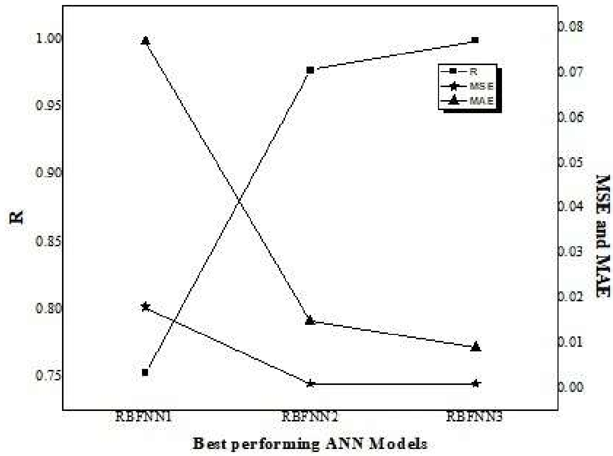

Fig. 4: Error statistics of RBFNN models during the testing period.

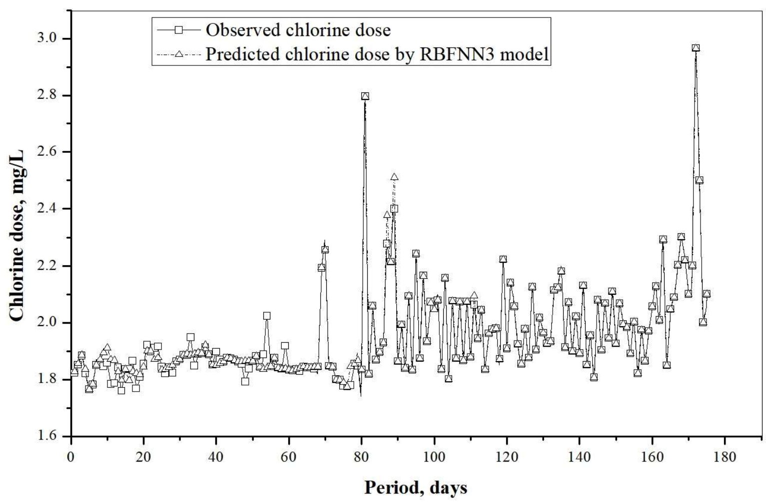

Fig. 4a: Time series of RBFNN3 model during the testing period.

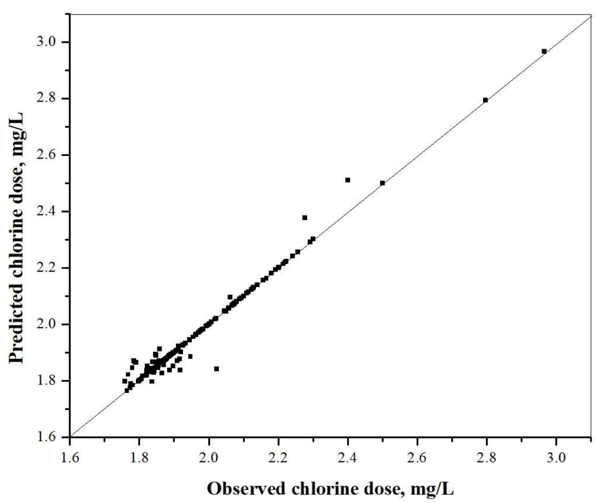

Fig. 4b: Scatter plot of RBFNN3 model during the testing period.

Development of Graphical User Interface

To transfer the modeling knowledge to the field, GUI software has been developed. The developed GUI will provide a useful tool to plant operators and managers for deciding the required chlorine and coagulant dose. GUIs for predicting chlorine dose in WTP were developed using the best model. The GUI was developed in MATLAB software. Determination of chlorine dose is an essential aspect of WTP. It decides the concentration of residual chlorine in the outgoing water of WTP. In India, most WTP operators provide higher chlorine doses for maintaining a high level of residual chlorine in WDN. The more chlorine consumption creates many health problems. Hence, there is a need to apply optimum chlorine dose. The GUI will be useful for the determination of chlorine dose at WTP.

1. Run the CCDNN model.
2. Enter the value of the coagulant dose applied at WTP in mg/L
3. Enter the value of outlet water turbidity (NTU)
4. Enter the value of desirable residual chlorine at the outlet of WTP so that minimum residual chlorine is maintained at the end of WDN.
5. After entering all data, click on the 'Chlorine Dose' button.
6. Within a few seconds, the chlorine dose value will be displayed in the output window (Fig 5).

Developed GUIs was helpful for WTP operators and managers to plan the short-term and long-term activities

CONCLUSION

Several CCDNN models have been developed to predict chlorine dosage, utilizing input parameters such as the outlet water's turbidity, residual chlorine, and coagulant dose for ANN modeling. These selected parameters are closely associated with chlorination and coagulation processes. As the concentration of suspended solids (SF) increases, the prediction efficiency of RBFNN and GRNN models decreases. However, within the RBFNN model, there is a noticeable superiority in prediction when SF ranges from 0.1 to 1. Such correlations prove valuable in determining the optimal chlorine or coagulant dosage. Additionally, it's observed that the range of chlorine dosage is narrower compared to that of the coagulant dosage. The relationship between them is established by the CCDNN model, wherein the prediction of chlorine dosage based on coagulant dosage demonstrated an impressive correlation (R = 0.99) according to RBFNN.

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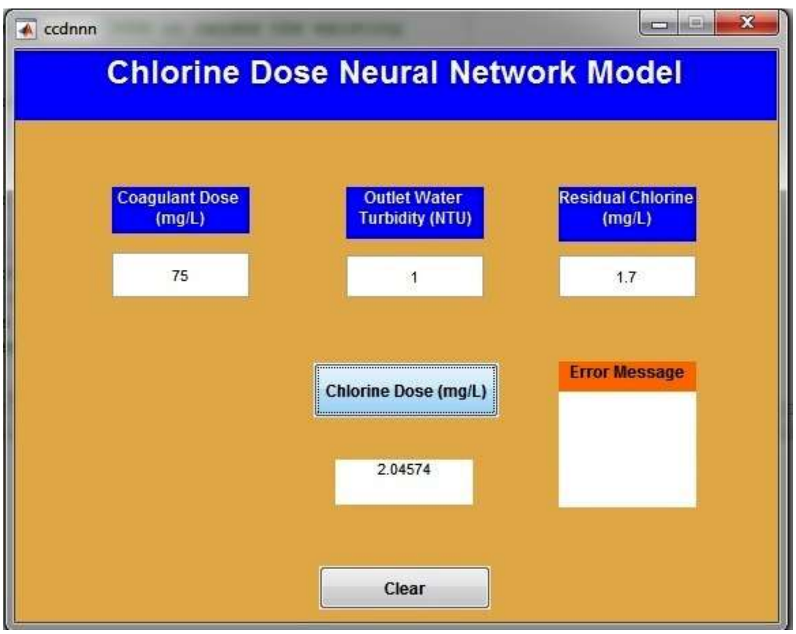

Fig. 5: Screen Shot of GUIfor CCDNN (RBNN3 (SF = 0.1)) model.

NOMENCLATURE

Symbol	Description
ANN	Artificial neural networks
ANFIS	Adaptive neural fuzzy inference system
BFGS	Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm
BR	Bayesian regularization
CFNN	Cascade feed forward neural network.
CDNN	Coagulant dose neural network
CCDNN	Coagulant and chlorine dose neural network
CGB	Conjugate gradient back propagation
FFNN	Feed forward neural network
GUI	Graphical user interface
GRNN	Generalized regression neural networks
GD	Gradient descent
GDM	Gradient descent with momentum
GCF	Conjugate gradient back propagation with Fletcher-Powell
LM	Levenberg-Marquardt
MAE	Mean absolute error
MSE	Mean square error
PCMC	Pimpri Chinchwad Municipal Corporation
RBFNN	Radial basis function neural network
RP	Resilient back propagation
RMSE	Root mean square error
R^2	Coefficient of determination
SF	Spread factor
WTP	Water treatment plant
WWTP	Wastewater treatment plant
WDN	Water distribution network
WQI	Water quality index

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